

10780391s2

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS	4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS	5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS	6	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS	7	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS	8	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS	9	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS	10	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS	11	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS	12	OCT 19	E-mail format enhanced
NEWS	13	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS	14	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	15	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	16	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	17	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	18	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS	19	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	20	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS	21	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS	22	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	23	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	24	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	25	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	26	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS	27	DEC 18	CA/CAplus patent kind codes updated
NEWS	28	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS	29	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	30	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS EXPRESS	NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.		

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NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8  
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:16:18 ON 05 JAN 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:16:29 ON 05 JAN 2007

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1

DICTIONARY FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

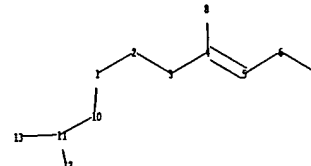
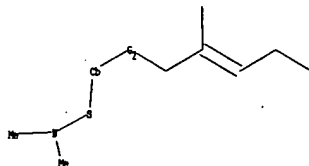
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10780391RTRs2.str

10780391s2



chain nodes :

1 2 3 4 5 6 7 8 10 11 12 13

chain bonds :

1-2 1-10 2-3 3-4 4-5 4-8 5-6 6-7 10-11 11-12 11-13

exact/norm bonds :

1-2 2-3 10-11

exact bonds :

1-10 3-4 4-5 4-8 5-6 6-7 11-12 11-13

G1:O,S

G2:O,S,N

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS

Element Count :

Node 1: Limited

C,C10

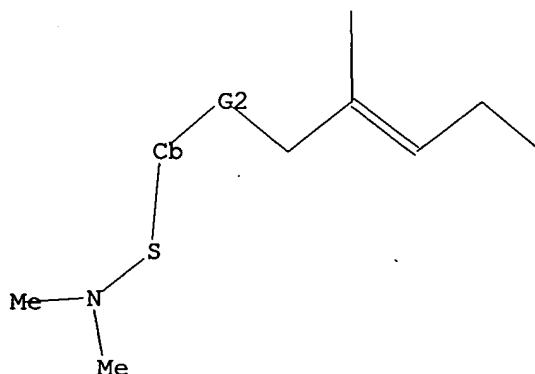
L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

10780391s2



G1 O,S

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:16:45 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 26 TO ITERATE

100.0% PROCESSED 26 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 215 TO 825

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 11:16:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 458 TO ITERATE

100.0% PROCESSED 458 ITERATIONS

11 ANSWERS

SEARCH TIME: 00.00.01

L3 11 SEA SSS FUL L1

=> fil hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'HCAPLUS' ENTERED AT 11:16:55 ON 05 JAN 2007

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FILE COVERS 1907 - 5 Jan 2007 VOL 146 ISS 3  
FILE LAST UPDATED: 4 Jan 2007 (20070104/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4                    2 L3

=> d ed ibib abs hitstr 1-2

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 05 Oct 2004  
 ACCESSION NUMBER: 2004:807711 HCAPLUS  
 DOCUMENT NUMBER: 142:6669  
 TITLE: Synthesis and Activity of Fluorescent Isoprenoid Pyrophosphate Analogs  
 AUTHOR(S): Kim, WeeKyung; Kleckley, Troy S.; Wiemer, Andrew J.; Holstein, Sarah A.; Mohl, Raymond J.; Wiemer, David F.  
 CORPORATE SOURCE: Departments of Chemistry Pharmacology and Internal Medicine, University of Iowa, Iowa City, IA, 52242-1294, USA  
 SOURCE: Journal of Organic Chemistry (2004), 69(24), 8186-8193  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 142:6669

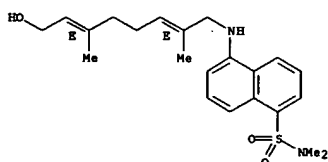
AB New fluorescent analogs of farnesol and geranylgeraniol were prepared and then converted to the corresponding pyrophosphates. These analogs incorporate anthranilate or dansyl-like groups anchored to the terpenoid skeleton through amine bonds that would be expected to be relatively stable to metabolism. After addition of the alcs. or the pyrophosphates to the culture medium, their fluorescence is readily observed inside a human-derived

leukemia cell line. Enzyme assays have revealed that the farnesyl pyrophosphate analog is an inhibitor of Ffase, while the corresponding alc. is not. These results, together with Western blot analyses of cell lysates, indicate that the farnesyl pyrophosphate analog penetrates the cells as an intact pyrophosphate and that it does so at a biol. relevant concentration.

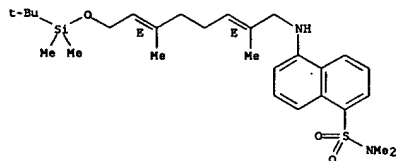
IT 491861-22-4P  
 RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents and inhibitors of farnesyl transferase)

RN 491861-22-4 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

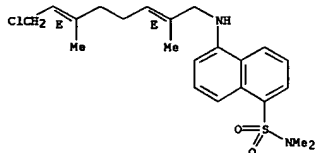


L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 798573-66-7 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-chloro-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

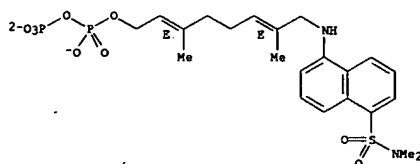


RN 798573-68-9 HCAPLUS  
 CN 1-Butanaminium, N,N,N-tributyl-, (2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl (diphosphate) (3:1) (9CI) (CA INDEX NAME)

CH 1

CRN 798573-67-8  
 CMF C22 H29 N2 O9 P2 S

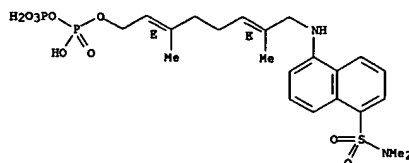
Double bond geometry as shown.



L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 798573-69-0P  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents and inhibitors of farnesyl transferase)  
 RN 798573-69-0 HCAPLUS  
 CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester, triammonium salt (9CI) (CA INDEX NAME)

Double bond geometry as shown.



●3 NH3

IT 798573-65-6P 798573-66-7P 798573-68-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

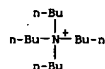
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents and inhibitors of farnesyl transferase)

RN 798573-65-6 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

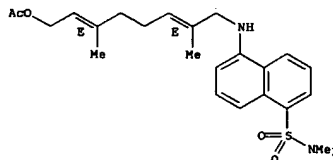
CH 2  
 CRN 10549-76-5  
 CMF C16 H36 N



IT 798573-64-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents and inhibitors of farnesyl transferase)

RN 798573-64-5 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-(acetoxymethyl)-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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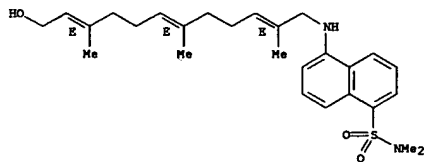
L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 31 Jan 2003  
 ACCESSION NUMBER: 2003:77548 HCAPLUS  
 DOCUMENT NUMBER: 138:142470  
 TITLE: Isoprenoid analog compounds and methods of making and use thereof  
 INVENTOR(S): Wiener, David; Hohl, Raymond J.  
 PATENT ASSIGNER(S): University of Iowa Research Foundation, USA  
 SOURCE: U.S. Pat. Appl. Publ., 18 pp.  
 CODEN: USXKCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003022869	A1	20030130	US 2002-116737	20020403
US 6727234	B2	20040427		
US 2004167102	A1	20040826	US 2004-780391	20040217
PRIORITY APPLN. INFO.:			US 2001-281170P	P 20010403
			US 2002-116737	A3 20020403

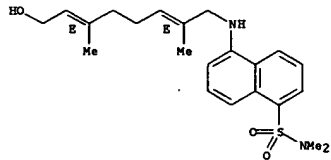
OTHER SOURCE(S): MARPAT 138:142470  
 AB The invention provides isoprenoid compds. and their pharmaceutically acceptable salts useful, for example, for blocking prenylation transferase enzymes, for probing or diagnosing protein prenylation processes, and for treating cancer in a mammal. A method of accessing the metabolic status of an enzyme comprises (a) contacting the enzyme with an effective amount of a mixture of a farnesol analog compound and a geraniol or geranylgeraniol analog compound, and (b) measuring the relative ratio of farnesylation to geranylgeranylation of the farnesol and the geraniol or geranylgeraniol analog compds. accomplished by the enzyme. The invention also provides pharmaceutical compds., and processes for preparing isoprenoid compds. and their intermediates.

IT 491861-20-2P  
 RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 RN 491861-20-2 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E,10E)-12-hydroxy-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

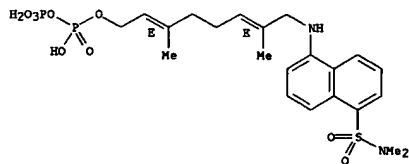


L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 491861-23-5 HCAPLUS  
 CN Diphosphoric acid, mono[(2E,6E)-9-[[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester (9CI) (CA INDEX NAME)

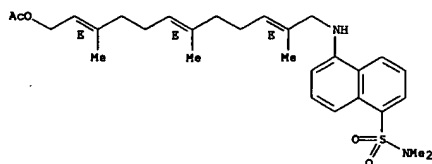
Double bond geometry as shown.



L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

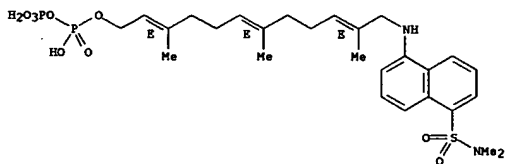
IT 491861-19-9P 491861-21-3P 491861-22-4P  
 491861-23-5P  
 RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 RN 491861-19-9 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E,10E)-12-(acetyloxy)-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 491861-21-3 HCAPLUS  
 CN Diphosphoric acid, mono[(2E,6E,10E)-12-[[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7,11-trimethyl-2,6,10-dodecatrienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 491861-22-4 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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=> fil reg

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
13.14	185.45
-1.56	-1.56

FILE 'REGISTRY' ENTERED AT 11:17:43 ON 05 JAN 2007  
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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1  
DICTIONARY FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

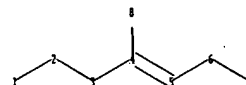
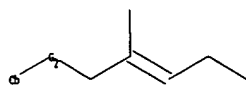
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and

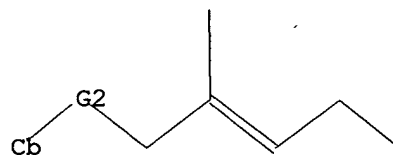


10780391s2



chain nodes :  
1 2 3 4 5 6 7 8  
chain bonds :

10780391s2



G1 O,S

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 11:18:25 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 12671 TO ITERATE

15.8% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 246676 TO 260164  
PROJECTED ANSWERS: 0 TO 0

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FILE COVERS 1907 - 5 Jan 2007 VOL 146 ISS 3  
FILE LAST UPDATED: 4 Jan 2007 (20070104/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17  
L8

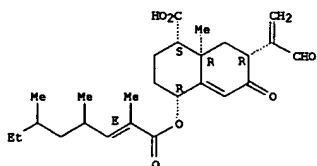
20 L7

=> d ed ibib abs hitstr 1-20

10780391s2

L8 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 05 Sep 2005  
 ACCESSION NUMBER: 2005:967021 HCAPLUS  
 DOCUMENT NUMBER: 144:208564  
 TITLE: New eremophilane-type sesquiterpenoids, eremoxylarins A and B from xylariaceae endophytic fungus YUA-026  
 AUTHOR(S): Shiono, Yoshitomo; Murayama, Tetsuya  
 CORPORATE SOURCE: Department of Bioresource Engineering, Faculty of Agriculture, Yamagata University, Tsuruoka, Yamagata, 997-8555, Japan  
 SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (2005), 60(8), 885-890  
 CODEN: ZNBSEN; ISSN: 0932-0776  
 PUBLISHER: Verlag der Zeitschrift fuer Naturforschung  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Two new eremophilane sesquiterpenes, eremoxylarins A and B, were isolated from the xylariaceae endophytic fungus YUA-026. Their structures were determined by spectroscopic methods. Eremoxylarins A and B showed antimicrobial activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa*.  
 IT 875760-50-2P, Eremoxylarin B  
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (new eremophilane-type sesquiterpenoids eremoxylarins A and B from xylariaceae endophytic fungus YUA-026 with antimicrobial activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa*)  
 RN 875760-50-2 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 7-[(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-4-[[[(2E)-2,4,6-trimethyl-1-oxo-2-octenyl]oxy]-, (1S,4R,7R,8aR)]- (9CI) (CA INDEX NAME)

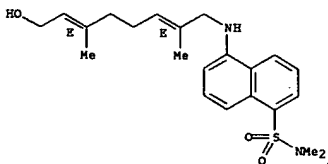
Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.  
 Currently available stereo shown.



IT 875760-52-4P, Eremoxylarin B methyl ester  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (new eremophilane-type sesquiterpenoids eremoxylarins A and B from xylariaceae endophytic fungus YUA-026 with antimicrobial activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa*)  
 RN 875760-52-4 HCAPLUS

L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 05 Oct 2004  
 ACCESSION NUMBER: 2004:807711 HCAPLUS  
 DOCUMENT NUMBER: 142:6669  
 TITLE: Synthesis and Activity of Fluorescent Isoprenoid Pyrophosphate Analogues  
 AUTHOR(S): Kim, MaeYoung; Kleckley, Troy S.; Wiemer, Andrew J.; Holstein, Sarah A.; Hohl, Raymond J.; Wiemer, David F.  
 CORPORATE SOURCE: Departments of Chemistry Pharmacology and Internal Medicine, University of Iowa, Iowa City, IA, 52242-1294, USA  
 SOURCE: Journal of Organic Chemistry (2004), 69(24), 8186-8193  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 142:6669  
 AB New fluorescent analogs of farnesol and geranylgeraniol were prepared and then converted to the corresponding pyrophosphates. These analogs incorporate anthranilate or dansyl-like groups anchored to the terpenoid skeleton through amine bonds that would be expected to be relatively stable to metabolism. After addition of the alcs. or the pyrophosphates to the culture medium, their fluorescence is readily observed inside a human-derived leukemia cell line. Enzyme assays have revealed that the farnesyl pyrophosphate analog is an inhibitor of Ffase, while the corresponding alc. is not. These results, together with Western blot analyses of cell lysates, indicate that the farnesyl pyrophosphate analog penetrates the cells as an intact pyrophosphate and that it does so at a biol. relevant concentration.  
 IT 491861-22-4P  
 RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents and inhibitors of farnesyl transferase)  
 RN 491861-22-4 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

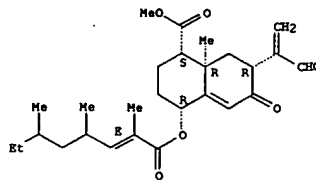
Double bond geometry as shown.



IT 798573-69-0P  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol

L8 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 CN 1-Naphthalenecarboxylic acid, 7-[(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-4-[[[(2E)-2,4,6-trimethyl-1-oxo-2-octenyl]oxy]-, methyl ester, (1S,4R,7R,8aR)]- (9CI) (CA INDEX NAME)

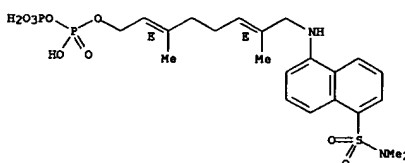
Absolute stereochemistry.  
 Double bond geometry as shown.  
 Currently available stereo shown.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 pyrophosphates as cellular imaging agents and inhibitors of farnesyl transferase)  
 RN 798573-69-0 HCAPLUS  
 CN Diphosphoric acid, mono[[[(2E,6E)-8-[[[5-[[[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester, triammonium salt (9CI) (CA INDEX NAME)

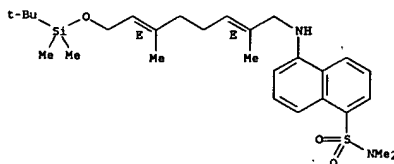
Double bond geometry as shown.



● 3 NH3

IT 798573-65-6P 798573-66-7P 798573-68-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents and inhibitors of farnesyl transferase)  
 RN 798573-65-6 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-[[[1,1-dimethylethyl]dimethylsilyl]oxy]-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

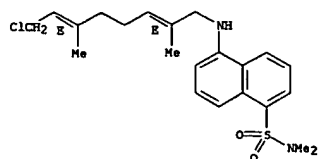


RN 798573-66-7 HCAPLUS  
 CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-chloro-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

10780391s2

L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

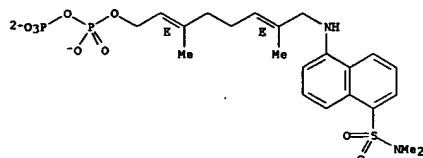


RN 798573-68-9 HCAPLUS  
 CN 1-Butanammonium, N,N,N-tributyl-, (2E,6E)-8-[[5-[[[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] diphosphate] (3:1) (9CI) (CA INDEX NAME)

CM 1

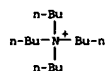
CRN 798573-67-8  
 CMF C22 H29 N2 O9 P2 S

Double bond geometry as shown.



CM 2

CRN 10549-76-5  
 CMF C16 H36 N



IT 798573-64-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents and inhibitors of farnesyl

L8 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 31 Jan 2003

ACCESSION NUMBER: 2003:77548 HCAPLUS

DOCUMENT NUMBER: 138:142470

TITLE: Isoprenoid analog compounds and methods of making and use thereof

INVENTOR(S): Wiemer, David; Hohl, Raymond J.

PATENT ASSIGNER(S): University of Iowa Research Foundation, USA

SOURCE: U.S. Pat. Appl. Publ., 18 pp.

DOCUMENT TYPE: CODEN: USXXCO

LANGUAGE: Patent

FAMILY ACC. NUM. COUNT: English

PATENT INFORMATION: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003022869	A1	20030130	US 2002-116737	20020403
US 6727234	B2	20040427		
US 2004167102	A1	20040826	US 2004-780391	20040217
			US 2001-281170P	P 20010403
			US 2002-116737	A3 20020403

OTHER SOURCE(S): MARPAT 138:142470

AB The invention provides isoprenoid compds. and their pharmaceutically acceptable salts useful, for example, for blocking prenylation transferase enzymes, for probing or diagnosing protein prenylation processes, and for treating cancer in a mammal. A method of accessing the metabolic status of an enzyme comprises (a) contacting the enzyme with an effective amount of a mixture of a farnesol analog compound and a geraniol or geranylgeraniol analog compound, and (b) measuring the relative ratio of farnesylation to geranylgeranylation of the farnesol and the geraniol or geranylgeraniol analog compds. accomplished by the enzyme. The invention also provides pharmaceutical compds., and processes for preparing isoprenoid compds. and their intermediates.

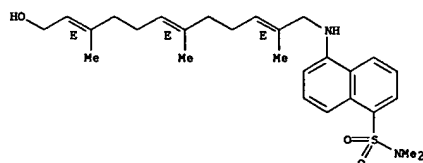
IT 491861-20-2P  
 RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(isoprenoid analog compds. for diagnosis and treatment of cancer)

RN 491861-20-2 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E,10E)-12-hydroxy-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 491861-19-9P 491861-21-3P 491861-22-4P  
 491861-23-5P

RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic

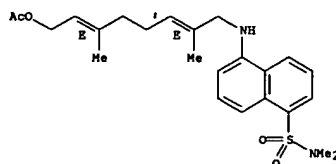
L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

transferase)

RN 798573-64-5 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-(acetyloxy)-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

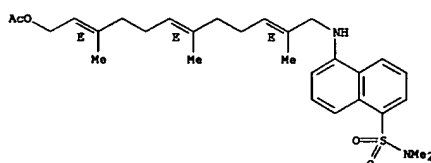
use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(isoprenoid analog compds. for diagnosis and treatment of cancer)

RN 491861-19-9 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E,10E)-12-(acetyloxy)-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

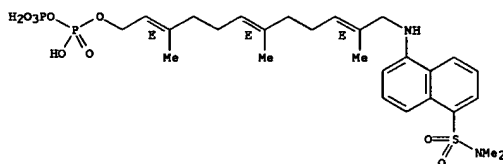
Double bond geometry as shown.



RN 491861-21-3 HCAPLUS

CN Diphosphoric acid, mono[(2E,6E,10E)-12-[[5-[[[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7,11-trimethyl-2,6,10-dodecatrienyl] ester] (9CI) (CA INDEX NAME)

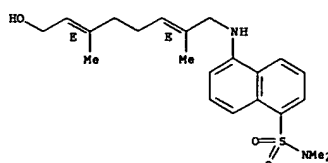
Double bond geometry as shown.



RN 491861-22-4 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

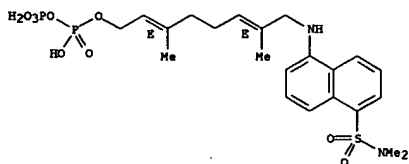
Double bond geometry as shown.



10780391s2

L8 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 RN 491861-23-5 HCAPLUS  
 CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



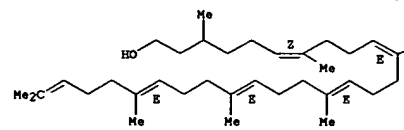
L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 10 Apr 2001  
 ACCESSION NUMBER: 2001:252486 HCAPLUS  
 DOCUMENT NUMBER: 135:19790

TITLE: Synthesis of dolichyl phosphates with a fluorescent label in the  $\gamma$ -isoprene unit of the chain  
 AUTHOR(S): Grigorieva, N. Ya.; Pinsker, O. A.; Mal'tsev, S. D.; Danilov, L. L.; Shibaev, V. N.; Jedrzejas, M. J.; N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 117913, Russia  
 CORPORATE SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2000), 49(12), 2065-2071  
 SOURCE: CODEN: RCBUEY; ISSN: 1066-5285  
 PUBLISHER: Consultants Bureau  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:19790

AB Stereoselective synthesis of the dolichyl phosphate derivs. WT3C2S-OP and WT2C6,7S-OP containing the 1-naphthylamino group in the  $\gamma$ -isoprene unit of the chain was performed. The synthetic scheme includes directed aldol condensation to construct (E)- $\alpha,\beta$ -disubstituted acroleins, their reductive amination with 1-aminonaphthalene, and phosphorylation of the resulting amino alcs.  
 IT 343311-91-1P 343312-11-8P 343312-12-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis of dolichyl phosphates with a fluorescent label)  
 RN 343311-91-1 HCAPLUS  
 CN 6,10,14,18,22,26-Octacosahexaen-1-ol, 3,7,15,19,23,27-hexamethyl-11-[(1-naphthalenylamino)methyl]-, (6Z,10E,14E,18E,22E)- (9CI) (CA INDEX NAME)

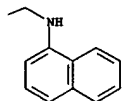
Double bond geometry as shown.

PAGE 1-A



L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

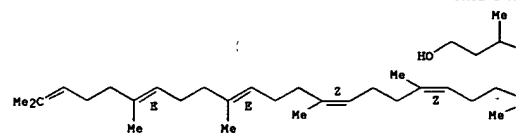
PAGE 1-B



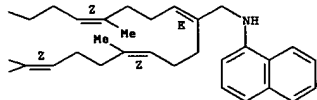
RN 343312-11-8 HCAPLUS  
 CN 6,10,14,18,22,26,30,34,38-Tetracontanonaen-1-ol, 3,7,15,19,23,27,31,35,39-nonamethyl-11-[(1-naphthalenylamino)methyl]-, (6Z,10E,14E,18E,22E,26E,30E,34E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

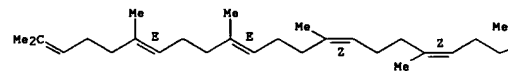


RN 343312-12-9 HCAPLUS  
 CN 6,10,14,18,22,26,30,34,38,42-Tetratetracontadecaen-1-ol, 3,7,15,19,23,27,31,35,39,43-decamethyl-11-[(1-naphthalenylamino)methyl]-, (6Z,10E,14E,18E,22E,26E,30E,34E,38E)- (9CI) (CA INDEX NAME)

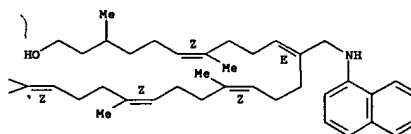
Double bond geometry as shown.

L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



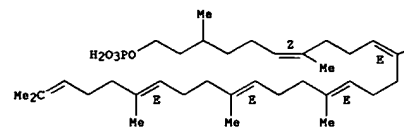
PAGE 1-B



IT 343311-92-2P 343311-99-9P 343312-00-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of dolichyl phosphates with a fluorescent label)  
 RN 343311-92-2 HCAPLUS  
 CN 6,10,14,18,22,26-Octacosahexaen-1-ol, 3,7,15,19,23,27-hexamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14E,18E,22E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

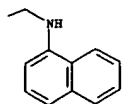


● 2 NH3

10780391s2

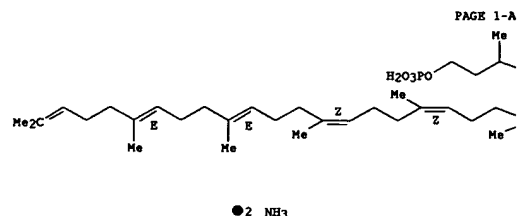
L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B



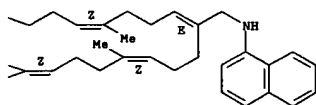
RN 343311-99-9 HCAPLUS  
 CN 6,10,14,18,22,26,30,34,38-Tetracontanonaen-1-ol, 3,7,15,19,23,27,31,35,39-nonamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14Z,18Z,22Z,26Z,30E,34E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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PAGE 1-B



RN 343312-00-5 HCAPLUS

L8 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 07 Dec 2000

ACCESSION NUMBER: 2000:857079 HCAPLUS

DOCUMENT NUMBER: 134:172483

TITLE: Ultrahigh pressure liquid chromatography/time-of-flight mass spectrometry for fast separations

AUTHOR(S): Wu, Haijun; Collins, David C.; Lippert, J. Andreas; Xiang, Yanqiao; Lee, Milton L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA

SOURCE: Journal of Microcolumn Separations (2000), 12(8), 462-469

CODEN: JMSEJ; ISSN: 1040-7685

PUBLISHER: John Wiley &amp; Sons, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Recently, ultraHPLC (UHPLC) was shown to overcome the pressure limitations that small particles impose on conventional pumping systems. High speed sepn. in UHPLC produce peak widths that range between 100 to 1000 ms, of which many are too narrow to be monitored by scanning mass spectrometers. The only mass spectrometer that is fast enough for such sepn. is the time-of-flight mass spectrometer (TOFMS). State-of-the-art TOFMS instruments for liquid chromatog. can record and store complete mass spectra at rates  $\leq 100$  spectra/s. High speed sepn. with high resolution were demonstrated using 13-15 cm  $\times$  29-100  $\mu$ m internal diameter capillaries packed with 1.5  $\mu$ m nonporous octadecylsilane- and isohexylsilane-modified silica particles using a home-built UHPLC system. The UHPLC system was successfully coupled to TOFMS via a liquid-sheath electrospray interface. Sepns. of selected combinatorial chemical samples, pharmaceutical compds., and herbicides were completed in  $<100$  s using UHPLC/TOFMS. Total column efficiencies ranged from 20,000-30,000 plates. The fundamental and practical aspects of UHPLC/TOFMS are discussed. Results are compared with those obtained from typical capillary LC.

IT 227302-93-4

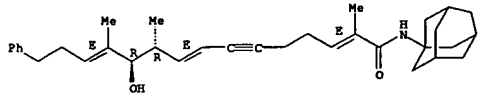
RI: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)  
 (ultrahigh pressure liquid chromatog./time-of-flight mass spectrometry for fast separation of combinatorial compds.)

RN 227302-93-4 HCAPLUS

CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-phenyl-N-tricyclo[3.3.1.3<sup>1,3</sup>]-dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



REFERENCE COUNT:

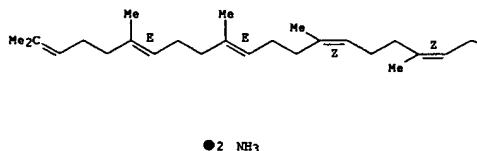
16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN 6,10,14,18,22,26,30,34,38,42-Tetratetracontadecaen-1-ol, 3,7,15,19,23,27,31,35,39,43-decamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14Z,18Z,22Z,26Z,30Z,34E,38E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 20 Jul 2000

ACCESSION NUMBER: 2000:490070 HCAPLUS

DOCUMENT NUMBER: 133:266274

TITLE: The Synthesis and Evaluation of a Solution Phase Indexed Combinatorial Library of Non-Natural Polyenes for Reversal of P-Glycoprotein Mediated Multidrug Resistance

AUTHOR(S): Andrus, Merritt B.; Turner, Timothy M.; Sauna, Zuben E.; Ambudkar, Suresh V.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA

SOURCE: Journal of Organic Chemistry (2000), 65(16), 4973-4983

CODEN: JOCEAH; ISSN: 0022-3263

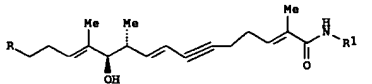
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:266274

GI



AB A combinatorial library of polyenes, based on (-)-stipiamide, has been constructed and evaluated for the discovery of new multidrug resistance reversal agents. A palladium coupling was used to react each individual vinyl iodide with a mixture of seven acetylenes at near 1:1 stoichiometry. The coupling was also used to react each individual acetylene with a mixture of six vinyl iodides to create 13 pools indexed in two dimensions for a total of 42 compds. Individual compds. were detected at equimolar concentration.

The vinyl iodides, made initially using a crotylborane addition to generate the anti-1,2-hydroxylmethyl products, were now made using a more efficient norephedrine propionate boron enolate aldol reaction. The indexed approach, ideally suited for cellular assays that involve membrane-bound targets, allowed for the rapid identification of reversal agents using assays with drug-resistant human breast cancer MCF7-adR cells. Intersections of potent pools identified new compds. with promising activity. Aryl dimension pools showed R = Ph and naphthyl as the most potent. The acetylene dimension had R = phenylalaninol and alaninol as the most potent. Isolated individual compds., both active and nonpotent, were assayed to confirm the library results. The most potent new compound was polyene I [R = 2-naphthyl, R1 = phenylalaninol] at 1.45  $\mu$ M. Other nonnatural individual naphthylamide compds. showed potent MDR reversal including I [R = 2-naphthyl, R1 = morpholinol] (1.69  $\mu$ M). Synergistic activities attributed to the two ends of the mol. were also identified. Direct interaction with Pgp was established by ATPase and photoaffinity displacement assays. The results indicate that both ends of the polyene reversal agent are involved in Pgp interaction and can be further modified for increased potency.

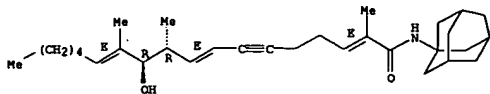
IT 227302-95-4P 227302-93-4P 227303-01-7P

227303-10-8P 227303-19-7P 227303-27-7P

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

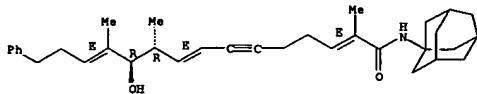
L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 study; PREP (Preparation)  
 (synthesis and evaluation of a soln. phase indexed combinatorial  
 library of non-natural polyenes for reversal of P-glycoprotein mediated  
 multidrug resistance)  
 RN 227302-85-4 HCAPLUS  
 CN 2,8,12-Octadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N-  
 tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



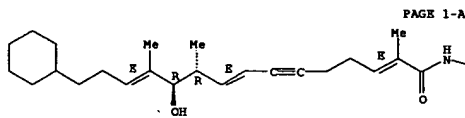
RN 227302-93-4 HCAPLUS  
 CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-phenyl-N-  
 tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



RN 227303-01-7 HCAPLUS  
 CN 2,8,12-Pentadecatrien-6-ynamide, 15-cyclohexyl-11-hydroxy-2,10,12-  
 trimethyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA  
 INDEX NAME)

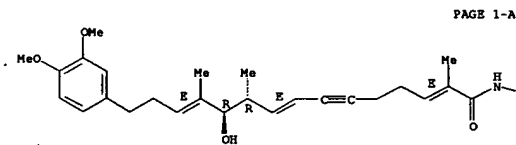
Absolute stereochemistry.  
 Double bond geometry as shown.



PAGE 1-A

L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 RN 227303-27-7 HCAPLUS  
 CN 2,8,12-Pentadecatrien-6-ynamide, 15-(3,4-dimethoxyphenyl)-11-hydroxy-  
 2,10,12-trimethyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



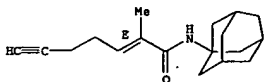
PAGE 1-A

PAGE 1-B



IT 227302-84-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (synthesis and evaluation of a solution phase indexed combinatorial  
 library of non-natural polyenes for reversal of P-glycoprotein mediated  
 multidrug resistance)  
 RN 227302-84-3 HCAPLUS  
 CN 2-Hepten-6-ynamide, 2-methyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E)- (9CI)  
 (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

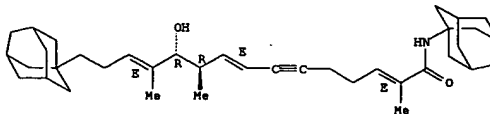
L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B



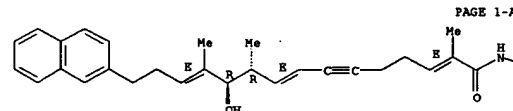
RN 227303-10-8 HCAPLUS  
 CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N,15-  
 bis(tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl)-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



RN 227303-19-7 HCAPLUS  
 CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-(2-  
 naphthalenyl)-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



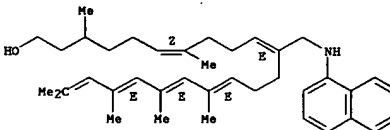
PAGE 1-A

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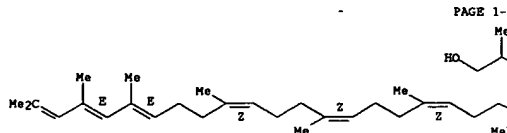
L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 19 Jun.2000  
 ACCESSION NUMBER: 2000:403626 HCAPLUS  
 DOCUMENT NUMBER: 133:252578  
 TITLE: Dolichyl phosphate derivatives with a fluorescent  
 label at an internal isoprene unit  
 AUTHOR(S): Grigorieva, Natalia Y.; Pinsky, Ol'ga A.; Maltsev,  
 Sergei D.; Danilov, Leonid L.; Shibaev, Vladimir N.;  
 Sedrezas, Mark J.  
 CORPORATE SOURCE: W.D. Zelinsky Institute of Organic Chemistry, Russian  
 Academy of Sciences, Moscow, 11913, Russia  
 SOURCE: Mendeleev Communications (2000), (3), 92-93  
 CODEN: MENCEX; ISSN: 0959-9436  
 PUBLISHER: Russian Academy of Sciences  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A general approach based on directed aldol condensation followed by  
 reductive amination with fluorescent amines and phosphorylation was  
 developed and illustrated by the synthesis of two dolichyl phosphate  
 derivs. with the 1-aminonaphthalene fluorophore at the γ-isoprene  
 unit of the chain.  
 IT 294846-40-5P 294846-48-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (Preparation of dolichyl phosphate derivs. with a fluorescent label at  
 internal isoprene unit)  
 RN 294846-40-5 HCAPLUS  
 CN 6,10,14,16,18,20-Docosahexaen-1-ol, 3,7,15,17,19,21-hexamethyl-11-[(1-  
 naphthalenylamino)methyl]-, (6Z,10E,14E,16E,18E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 294846-48-3 HCAPLUS  
 CN 5,9,13,17,21,25,29,33,35,37-Nonatriacontadecaen-1-ol,  
 2,6,14,18,22,26,30,34,36,38-decamethyl-10-[(1-naphthalenylamino)methyl]-,  
 (5Z,9E,13Z,17Z,21Z,25Z,29Z,33E,35E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



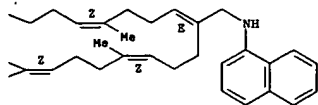
PAGE 1-A



10780391s2

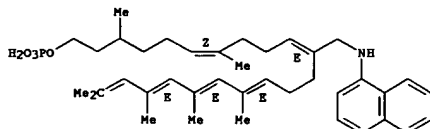
L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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IT 294846-41-6P 294846-44-9P 294846-45-0P  
 294846-49-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of dolichyl phosphate derivs. with a fluorescent label at  
 internal isoprene unit)  
 RN 294846-41-6 HCAPLUS  
 CN 6,10,14,18,20-Docosahexaen-1-ol, 3,7,15,17,19,21-hexamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14E,16E,18E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

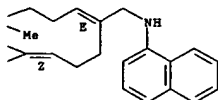
● 2 NH<sub>3</sub>

RN 294846-44-9 HCAPLUS  
 CN 5,9,13,17,21,25,29,31,33-Pentatriacontanonaen-1-ol, 2,6,14,18,22,26,30,32,34-nonamethyl-10-[(1-naphthalenylamino)methyl]-, (5Z,9E,13Z,17Z,21Z,25Z,29E,31E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

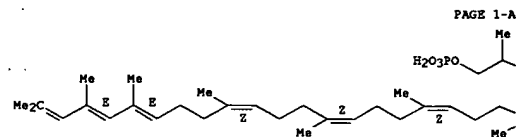
L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B

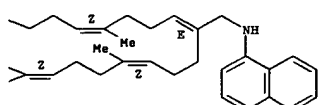


RN 294846-49-4 HCAPLUS  
 CN 6,10,14,18,22,26,30,34,36,38-Tetracontadecaen-1-ol, 3,7,15,19,23,27,31,35,37,39-decamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14Z,18Z,22Z,26Z,30Z,34E,36E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

● 2 NH<sub>3</sub>

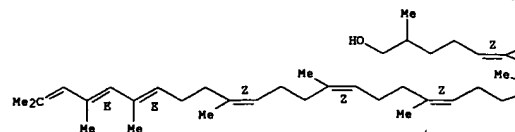
PAGE 1-B



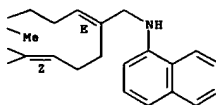
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



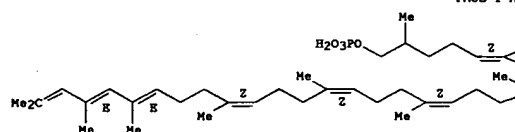
PAGE 1-B



RN 294846-45-0 HCAPLUS  
 CN 5,9,13,17,21,25,29,31,33-Pentatriacontanonaen-1-ol, 2,6,14,18,22,26,30,32,34-nonamethyl-10-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (5Z,9E,13Z,17Z,21Z,25Z,29E,31E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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● 2 NH<sub>3</sub>

L8 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 10 May 2000

ACCESSION NUMBER: 2000:303525 HCAPLUS

DOCUMENT NUMBER: 133:89286

TITLE: Symmetrically-substituted decalin-based scaffolds  
 Plyta, Zoi F.; Heller, Eberhard; Dumas, Francoise;  
 Miet, Christine; Mahuteau, Jacqueline; d'Angelo, Jean;

CORPORATE SOURCE: Caturla, Juen; Dau, Marie-Elise Tran Huu  
 Centre d'Etudes Pharmaceutiques, Université de Paris  
 Sud, Laboratoire de Synthèse Organique, BIOICIS, Unité  
 associée au CNRS 5, Chateaufort-Malabry, 92296, Fr.

SOURCE: Tetrahedron Letters (2000), 41(16), 2907-2910

CODEN: TETLEA; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of a chiral scaffold was achieved by coupling  
 (2R,7S)-rel-4a-[[[(1,1-dimethylethyl)phenylsilyl]oxy]methyl]decahydro-2,7-  
 naphthalenediol with (2E,4S)-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-  
 methyl-2-pentenoic acid. The target compound was (2E,4S)-4-[[[(1,1-  
 dimethylethoxy)carbonyl]amino]-2-methyl-2-pentenoic acid  
 (2R,7S)-4a-[[[(1,1-Dimethylethyl)phenylsilyl]oxy]methyl]decahydro-2,7-  
 naphthalenediyl ester. The two side chains of this mol. strongly  
 self-associate through intramol. hydrogen bonding involving the NH-BOC  
 residues. The Mosher ester analog of the above decalin derivative was also  
 prepared; (4R)-α-methoxy-α-(trifluoromethyl)benzeneacetic  
 acid (2R,7S)-4a-[[[(1,1-Dimethylethyl)phenylsilyl]oxy]methyl]decahydro-2,7-  
 naphthalenediyl ester.

IT 281193-88-2

RL: PRP (Properties)

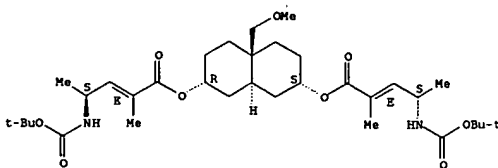
(preparation and properties of [(dimethylethoxy)carbonyl]amino]pentenoic  
 acid [(silyloxy)methyl]decahydronaphthalenediyl ester)

RN 281193-88-2 HCAPLUS

CN 2-Pentenoic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-methyl-,  
 (2α,4αβ,7α,8α)-decahydro-4a-(methoxymethyl)-2,7-  
 naphthalenediyl ester, (2E,2'E,4R,4'R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



IT 281193-86-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and properties of [(dimethylethoxy)carbonyl]amino]pentenoic  
 acid [(silyloxy)methyl]decahydronaphthalenediyl ester)

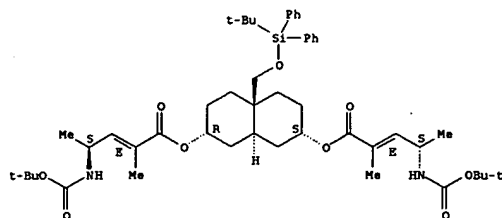
RN 281193-86-0 HCAPLUS

CN 2-Pentenoic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-methyl-,  
 (2α,4αβ,7α,8α)-4a-[[[(1,1-

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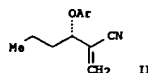
L8 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 dimethylethyl)diphenylsilyl]oxy)methyl]decahydro-2,7-naphthalenediyl  
 ester, (2E,2'E,4R,4'R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.

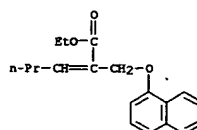


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 24 Mar 2000  
 ACCESSION NUMBER: 2000:188799 HCAPLUS  
 DOCUMENT NUMBER: 133:4276  
 TITLE: Deracemization of Baylis-Hillman Adducts  
 AUTHOR(S): Trost, Barry M.; Tsui, Hon-Chung; Toste, F. Dean  
 CORPORATE SOURCE: Department of Chemistry, Stanford University,  
 Stanford, CA, 94305-5080, USA  
 SOURCE: Journal of the American Chemical Society (2000),  
 122(14), 3534-3535  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 133:4276  
 GI

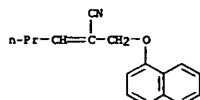


AB Pd2dba3 in presence of a chiral ligand catalyzed the reaction of phenols  
 with carbonates of Baylis-Hillman adducts RCH(OCO2Me)C(EWG):CH2 (I; R =  
 Pr, PhCH2CH2, etc.; EWG = CN, CO2Et).  
 IT 270903-55-4F 270903-56-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (deracemization of Baylis-Hillman adducts)  
 RN 270903-55-4 HCAPLUS  
 CN 2-Hexenoic acid, 2-[(1-naphthalenyloxy)methyl]-, ethyl ester (9CI) (CA  
 INDEX NAME)



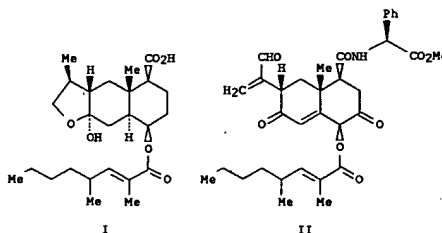
RN 270903-56-5 HCAPLUS  
 CN 2-Hexenenitrile, 2-[(1-naphthalenyloxy)methyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

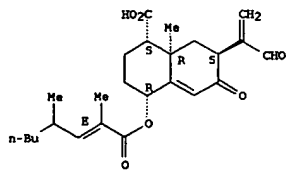
L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 05 Mar 2000  
 ACCESSION NUMBER: 2000:146880 HCAPLUS  
 DOCUMENT NUMBER: 132:308514  
 TITLE: Chemical and enzymatic modifications of integrase acid  
 and HIV-1 integrase inhibitory activity  
 AUTHOR(S): Singh, Sheo B.; Felock, Peter; Hazuda, Daria J.  
 CORPORATE SOURCE: Natural Products Drug Discovery, Merck Research  
 Laboratories, Rahway, NJ, 07065, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2000),  
 10(3), 235-238  
 CODEN: BMCLEB; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Integric acid, an acyl eremophilane sesquiterpenoid, was identified as an  
 inhibitor of HIV-1 integrase, the enzyme responsible for provirus entry  
 into the host cell nucleus and integration in to the host genome. Chemical  
 and enzymic modification of integric acid led to the preparation of several  
 selective chemical derivs., e.g. I and II, of integric acid. Preparation,  
 HIV-1 inhibitory activity, and the structure-activity relationship against  
 coupled and strand transfer assays are described. It appears that most of  
 the groups present in the natural product are required for inhibition of  
 HIV-1 integrase strand transfer activity. In contrast, inhibition of 3'  
 processing activity is less stringent suggesting distinct SAR for the two  
 integrase reactions.  
 IT 215866-65-2, Integrac acid  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); RCT (Reactant); BIOL (Biological study); RACT  
 (Reactant or reagent)  
 (chemical and enzymic modifications of integric acid and HIV-1 integrase  
 inhibitory activity)  
 RN 215866-65-2 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-  
 (1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-,  
 (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
Double bond geometry as shown.  
Currently available stereo shown.

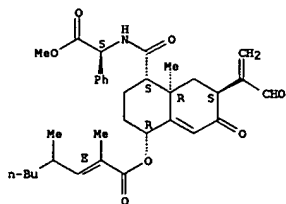


IT 254976-47-1P 254976-48-2P 264255-62-1P  
264255-63-2P 264255-65-4P 264255-68-7P  
264255-69-8P 264255-71-2P 264255-72-3P  
264255-73-4P 264255-74-5P 264255-75-6P  
264255-76-7P 264255-77-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREF (Preparation)  
(chemical and enzymic modifications of integrase acid and HIV-1 integrase inhibitory activity)

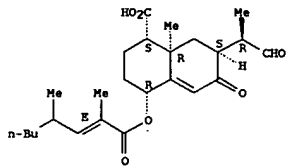
RN 254976-47-1 HCAPLUS  
CN Benzenecarboxylic acid, 4-[[[(1S,4R,7S,8aR)-4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.  
Currently available stereo shown.



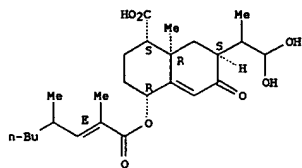
RN 254976-48-2 HCAPLUS  
CN Benzenecarboxylic acid, 4-[[[(1S,4R,7S,8aR)-4-[[[(2E)-2,4-dimethyl-1-oxo-

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



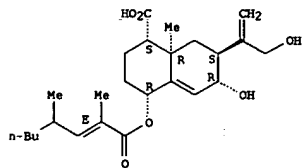
RN 264255-65-4 HCAPLUS  
CN 1-Naphthalenecarboxylic acid, 7-[(2,2-dihydroxy-1-methylethyl)-4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 264255-68-7 HCAPLUS  
CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-6-hydroxy-7-[(1-hydroxymethyl)ethenyl]-8a-methyl-, (1S,4R,6R,7S,8aR)- (9CI) (CA INDEX NAME)

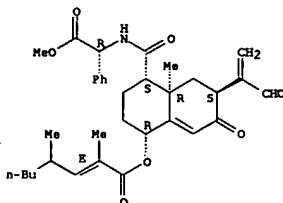
Absolute stereochemistry.  
Double bond geometry as shown.



RN 264255-69-8 HCAPLUS

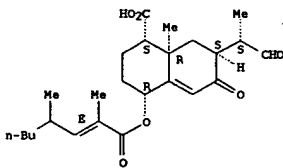
L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.  
Currently available stereo shown.



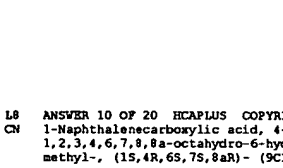
RN 264255-62-1 HCAPLUS  
CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-[(1S)-1-methyl-2-oxoethyl]-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



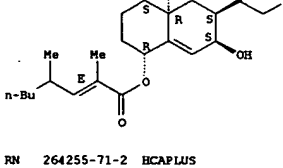
RN 264255-63-2 HCAPLUS  
CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-[(1R)-1-methyl-2-oxoethyl]-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



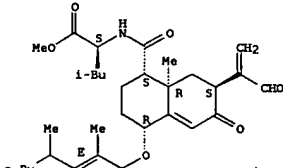
RN 264255-71-2 HCAPLUS  
CN 2-Octenoic acid, 2,4-dimethyl-, (1R,4S,4aR,6S)-6-(1-formylethenyl)-1,2,3,4,4a,5,6,7-octahydro-4-[[[(1S)-1-(methoxycarbonyl)-3-methylbutyl]amino]carbonyl]-4a-methyl-7-oxo-1-naphthalenyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 264255-72-3 HCAPLUS  
CN 2-Octenoic acid, 2,4-dimethyl-, 1,4-piperazinediylbis[carbonyl]-(1R,4S,4aR,6S)-6-(1-formylethenyl)-1,2,3,4,4a,5,6,7-octahydro-4a-methyl-7-oxo-4,1-naphthalenediyl] ester, (2E,2'E)- (9CI) (CA INDEX NAME)

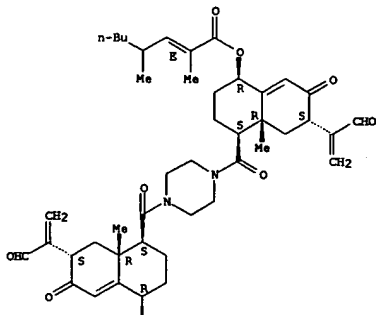
Absolute stereochemistry.  
Double bond geometry as shown.



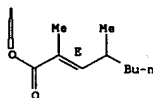
RN 264255-73-3 HCAPLUS  
CN 2-Octenoic acid, 2,4-dimethyl-, 1,4-piperazinediylbis[carbonyl]-(1R,4S,4aR,6S)-6-(1-formylethenyl)-1,2,3,4,4a,5,6,7-octahydro-4a-methyl-7-oxo-4,1-naphthalenediyl] ester, (2E,2'E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

PAGE 1-A



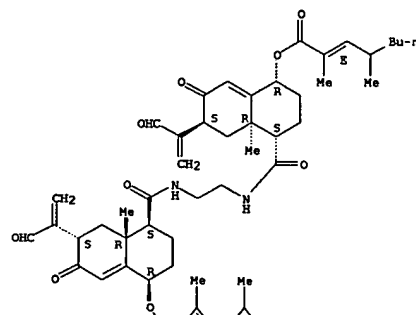
PAGE 2-A



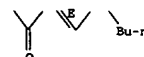
RN 264255-73-4 HCAPLUS  
 CN 2-Octenoic acid, 2,4-dimethyl-, 1,2-ethanediylbis[iminocarbonyl] [(1R,4S,4aR,6S)-6-[(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-oxo-4,1-naphthalenediyl]] ester, (2E,2'E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

PAGE 1-A

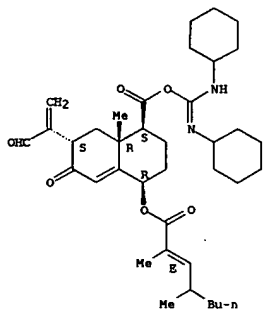


PAGE 2-A



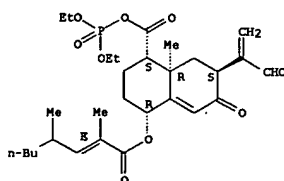
RN 264255-74-5 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, anhydride with N,N'-dicyclohexylcarbamidic acid, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



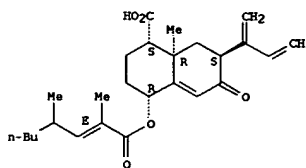
RN 264255-75-6 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, anhydride with diethyl hydrogen phosphate, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



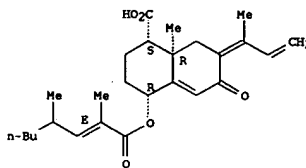
RN 264255-76-7 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-(1-methylene-2-propenyl)-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



RN 264255-77-8 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-(1-methyl-2-propenylidene)-6-oxo-, (1S,4R,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as described by E or Z.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10780391s2

L8 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 09 Dec 1999

ACCESSION NUMBER: 1999:777604 HCAPLUS

DOCUMENT NUMBER: 132:90477

TITLE: Structure and absolute stereochemistry of HIV-1 integrase inhibitor integric acid, a novel eremophilane sesquiterpenoid produced by a *Xylaria* sp. Singh, Sheo B.; Zink, Deborah; Polishook, Jon; Valentino, Delia; Shafiee, Ali; Silverman, Keith; Felock, Peter; Teran, Ana; Vilella, Dolores; Hazuda, Daria J.; Lingham, Russell B.

CORPORATE SOURCE: Natural Products Drug Discovery, Merck Research Laboratories, Rahway, NJ, 07065, USA

SOURCE: Tetrahedron Letters (1999), 40(150), 8775-8779

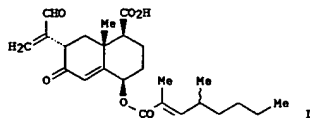
CODEN: TETLEA; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB HIV-1 integrase is critical for viral replication and is absent in the host, and therefore is a potential target for the development of non-toxic antiviral therapy. Integrac acid (I), a novel eremophilane sesquiterpenoid, was isolated from the fermentation broth of *Xylaria* sp. (MF6254). I inhibited 3'-end processing, strand transfer and disintegration reactions catalyzed by HIV-1 integrase with IC50 values of 3-10  $\mu$ M. The isolation, structure elucidation, relative, and absolute stereochemistry of integric acid were described.

IT 215866-65-2P, (+)-Integrac acid

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MPH (Metabolic formation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)

(isolation, mol. structure, absolute configuration, and HIV-1 integrase inhibiting activity of integric acid, a novel eremophilane sesquiterpenoid metabolite of *Xylaria* sp. (MF6254))

RN 215866-65-2 HCAPLUS

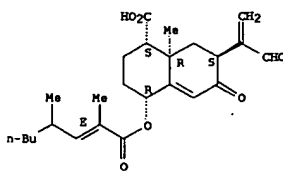
CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.

L8 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 215866-73-2P, (+)-Integrac acid methyl ester 254976-47-1P

254976-48-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (isolation, mol. structure, absolute configuration, and HIV-1 integrase inhibiting activity of integric acid, a novel eremophilane sesquiterpenoid metabolite of *Xylaria* sp. (MF6254))

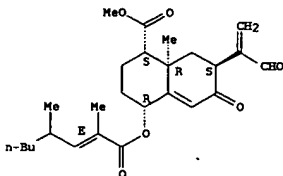
RN 215866-73-2 HCAPLUS

CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, methyl ester, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.



RN 254976-47-1 HCAPLUS

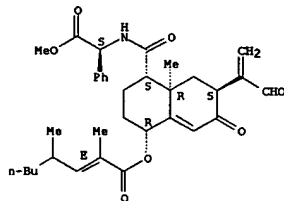
CN Benzeneacetic acid,  $\alpha$ -[[[(1S,4R,7S,8aR)-4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.

L8 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



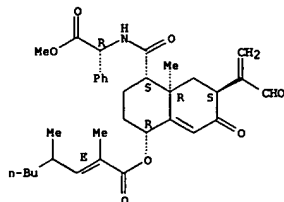
RN 254976-48-2 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[[[(1S,4R,7S,8aR)-4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

Currently available stereo shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 22 Apr 1999

ACCESSION NUMBER: 1999:246151 HCAPLUS

DOCUMENT NUMBER: 131:70216

TITLE: Isolation and characterization of novel human immunodeficiency virus integrase inhibitors from fungal metabolites

AUTHOR(S): Hazuda, Daria; Blau, Carol; Uncapher, Felock, Peter; Hastings, Jeffrey; Pramanik, Bernali; Wolfe, Abigail; Bushman, Frederick; Farnet, Chris; Goetz, Michael; Williams, Marie; Silverman, Keith; Lingham, Russell; Singh, Sheo

CORPORATE SOURCE: Department of Antiviral Research, Merck Research Laboratories, West Point, PA, 19486, USA

SOURCE: Antiviral Chemistry & Chemotherapy (1999), 10(2), 63-70

CODEN: ACCHEH; ISSN: 0956-3202

PUBLISHER: International Medical Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have identified a series of novel inhibitors of human immunodeficiency virus type 1 (HIV-1) integrase by randomly screening natural product extracts using an in vitro biochem. assay designed to identify inhibitors of integrase-catalyzed strand transfer. Equisetin recovered from the fungus *Fusarium heterosporum* and a novel enantiomeric homolog of equisetin from *Phoma* sp. were isolated as inhibitors of HIV-1 integrase in vitro. Two additional analogs, a novel decalin derivative, integrac acid, and oteromycin

were also discovered to be inhibitors of integrase. Equisetin and related compounds inhibit 3' end-processing and strand transfer as well as disintegration catalyzed by either the full-length enzyme or the truncated integrase core domain (amino acids 50-212). These compounds also inhibit strand transfer reactions catalyzed by stable complexes assembled in vitro and integration reactions catalyzed by pre-integration complexes isolated from HIV-1-infected cells. The compounds described in this report are structurally novel and mechanistically distinct from many previously described inhibitors of HIV-1 integrase. These results demonstrate the utility of using an appropriately configured assay to identify compounds that are effective post-assembly and the potential of isolating novel integrase inhibitors from complex natural product extracts.

IT 215866-65-2P, Integrac acid

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (isolation and characterization of novel human immunodeficiency virus integrase inhibitors from fungal metabolites)

RN 215866-65-2 HCAPLUS

CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

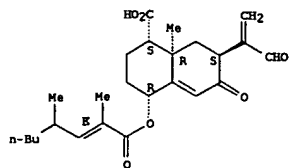
Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.

10780391s2

L8 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 16 Apr 1999

ACCESSION NUMBER: 1999:234630 HCAPLUS

DOCUMENT NUMBER: 131:44674

TITLE: The Synthesis and Evaluation of a Solution-Phase Indexed Combinatorial Library of Non-natural Polyenes. for Multidrug Resistance Reversal

AUTHOR(S): Andrus, Merritt B.; Turner, Timothy M.; Asgari, Davoud; Li, Wenke

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA

SOURCE: Journal of Organic Chemistry (1999), 64 (9), 2978-2979

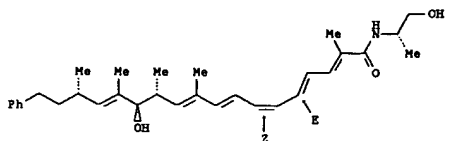
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB A solution-phase library, based on the multidrug resistance reversing polyene, (-)-stipiamide (1), that consists of mixts. indexed in two dimensions that provides for efficient combinatorial synthesis, direct screening with a cellular assay, and the isolation and testing of individual compds. is reported.

IT 227302-85-4P 227302-93-4P 227303-01-7P

227303-10-8P 227303-19-7P 227303-27-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and evaluation of a solution-phase combinatorial library of non-natural polyenes for multidrug resistance reversal)

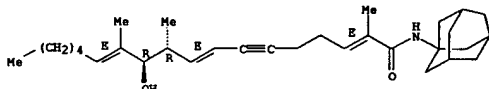
RN 227302-85-4 HCAPLUS

CN 2,8,12-Octadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L8 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

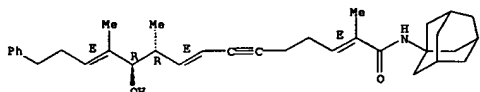


RN 227302-93-4 HCAPLUS

CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-phenyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

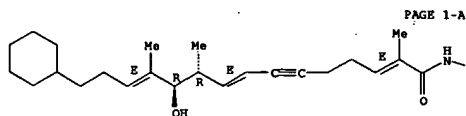


RN 227303-01-7 HCAPLUS

CN 2,8,12-Pentadecatrien-6-ynamide, 15-cyclohexyl-11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



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PAGE 1-B

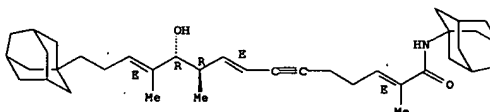
RN 227303-10-8 HCAPLUS

CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N-bis(tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl)-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.

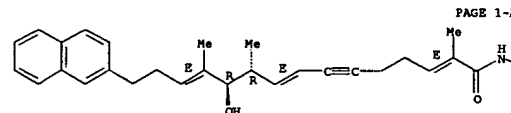


RN 227303-19-7 HCAPLUS

CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-(2-naphthalenyl)-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



PAGE 1-A



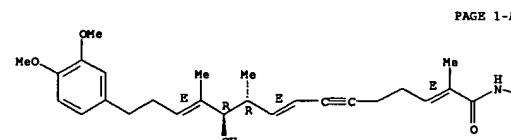
PAGE 1-B

RN 227303-27-7 HCAPLUS

CN 2,8,12-Pentadecatrien-6-ynamide, 15-(3,4-dimethoxyphenyl)-11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

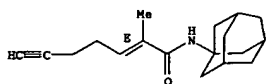


PAGE 1-A



IT 227302-84-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (synthesis and evaluation of a solution-phase combinatorial library of  
 non-natural polyenes for multidrug resistance reversal)  
 RN 227302-84-3 HCAPLUS  
 CN 2-Hepten-6-ynamide, 2-methyl-N-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, (2E)- (9CI)  
 (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ED Entered STN: 22 Jan 1999

ACCESSION NUMBER: 1999:45072 HCAPLUS

DOCUMENT NUMBER: 130:119582

TITLE: Ermophilane sesquiterpenoids as HIV integrase

inhibitors

INVENTOR(S): Lingham, Russell B.; Polishook, Jon David; Shafiee,  
 Ali; Silverman, Keith C.; Singh, Sheo Bux; Zink,  
 Deborah L.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: U.S., 10 pp.

DOCUMENT TYPE: CODEN: USOXAM

LANGUAGE: Patent

FAMILY ACC. NUM. COUNT: English

PATENT INFORMATION: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5858738	A	19990112	US 1997-964081	19971104
PRIORITY APPL. INFO.: US 1997-964081 19971104				

OTHER SOURCE(S): MARPAT 130:119582

AB Natural products such as certain ermophilane sesquiterpenoids and derivs.  
 thereof are described. These compds. are useful in the inhibition of HIV  
 integrase, the prevention or treatment of infection by HIV and the  
 treatment of AIDS, either as compds., pharmaceutically acceptable salts,  
 pharmaceutical composition ingredients, whether or not in combination with  
 other antivirals, immunomodulators, antibiotics or vaccines. Methods of  
 treating AIDS and methods of preventing or treating infection by HIV are  
 also described. The fungal culture MF6254, Xylaria sp. (ATCC 74397) is  
 also described and disclosed.

IT 215866-65-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); PUR (Purification or recovery); RCT (Reactant); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT  
 (Reactant or reagent); USES (Uses)  
 (ermophilane sesquiterpenoids as HIV integrase inhibitors)

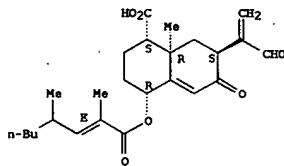
RN 215866-65-2 HCAPLUS

CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-  
 (1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-,  
 (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.

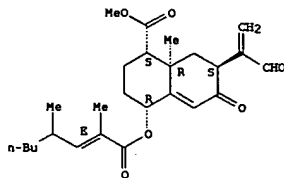


IT 215866-73-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
 BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (ermophilane sesquiterpenoids as HIV integrase inhibitors)  
 RN 215866-73-2 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-  
 (1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, methyl  
 ester, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.



IT 215866-65-2D, esters  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES  
 (Uses)  
 (ermophilane sesquiterpenoids as HIV integrase inhibitors)

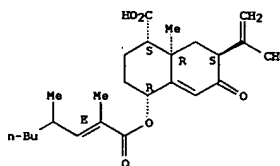
RN 215866-65-2 HCAPLUS

CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-  
 (1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-,  
 (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.



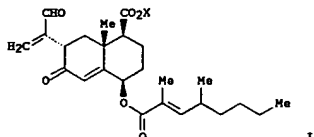
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10780391s2

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 18 Dec 1998  
 ACCESSION NUMBER: 1998:791573 HCAPLUS  
 DOCUMENT NUMBER: 130:10607  
 TITLE: HIV integrase inhibitors from culture of Xylaria species  
 INVENTOR(S): Lingham, Russell B.; Polishook, Jon D.; Shafiee, Ali; Silverman, Keith C.; Singh, Sheo B.; Zink, Deborah L.  
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA  
 SOURCE: Brit. UK Pat. Appl., 35 pp.  
 CODEN: BAOXDU  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2319026	A	19980513	GB 1997-22761	19971028
PRIORITY APPLN. INFO.:			GB 1997-22761	A 19971028
			GB 1996-25326	P 19961205
			US 1996-29886P	19961107

OTHER SOURCE(S): MARPAT 130:10607  
 GI

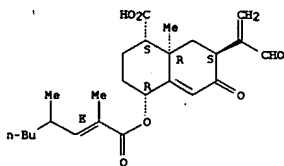


AB Natural products such as certain eremophilane sesquiterpenoids and derivs., useful in the inhibition of HIV integrase, the prevention or treatment of infection by HIV and the treatment of AIDS, ether as compds., pharmaceutically acceptable salts, pharmaceutical composition ingredients, whether or not in combination with other antivirals, immunomodulators, antibiotics, or vaccines are described. The compds. (I; X = H, (substituted) C1-14 alkyl) are isolated from a novel fungal culture MF6254, Xylaria sp. (ATCC 74397).

IT 215866-65-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (HIV integrase inhibitors from culture of Xylaria species)  
 RN 215866-65-2 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

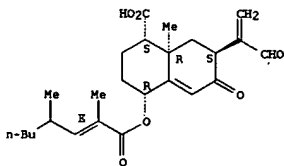
L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.  
 Currently available stereo shown.



RN 215866-69-6 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, calcium salt, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.  
 Currently available stereo shown.

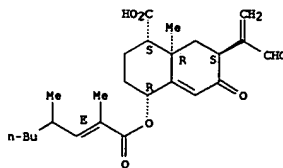


RN 215866-70-9 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2,4-dimethyl-1-oxo-2-octenyl]oxy)-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1R,4S,7R,8aS)-rel-, compd. with 1,2-ethanediamine (1:1) (9CI) (CA INDEX NAME)

CH 1

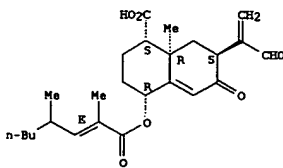
CRN 215866-65-2  
 CMF C25 H34 O6

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.  
 Currently available stereo shown.



IT 215866-66-3P 215866-67-4P 215866-69-6P  
 215866-70-9P 215866-71-0P 215866-72-1P  
 215866-73-2P 215866-74-3P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (HIV integrase inhibitors from culture of Xylaria species)  
 RN 215866-66-3 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, ammonium salt, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

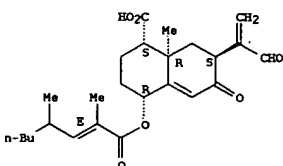
Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.  
 Currently available stereo shown.



RN 215866-67-4 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, potassium salt, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.  
 Currently available stereo shown.



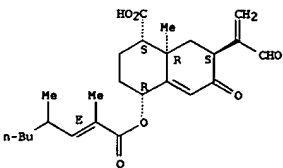
CH 2  
 CRN 107-15-3  
 CMF C2 H8 N2

H2N-CH2-CH2-NH2

RN 215866-71-0 HCAPLUS  
 CN 1-Naphthalenecarboxylic acid, 4-[[[(2,4-dimethyl-1-oxo-2-octenyl]oxy)-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1R,4S,7R,8aS)-rel-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CH 1  
 CRN 215866-65-2  
 CMF C25 H34 O6

Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.  
 Currently available stereo shown.

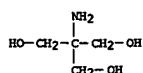


CH 2

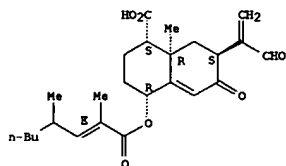


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L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 77-86-1  
CMP C4 H11 N O3RN 215866-72-1 HCAPLUS  
CN L-lysine, mono[rel-(1R,4S,7R,8aS)-4-[(2,4-dimethyl-1-oxo-2-octenyl)oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenecarboxylate] (9CI) (CA INDEX NAME)

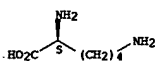
CM 1

CRN 215866-65-2  
CMP C25 H34 O6Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.  
Currently available stereo shown.

CM 2

CRN 56-87-1  
CMP C6 H14 N2 O2

Absolute stereochemistry.

RN 215866-73-2 HCAPLUS  
CN 1-Naphthalenecarboxylic acid, 4-[[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-

L8 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 28 May 1994

ACCESSION NUMBER: 1994:270951 HCAPLUS

DOCUMENT NUMBER: 120:270951

TITLE: Total synthesis of (+)-13-ethyl-3-methoxygonal, 3,5,9(11)-tetraen-17-one via the tandem Claisen-ene strategy  
Green-Piotrowska, E. M.; Green, M. B.  
Organon Sci. Dev. Group, Oas, 5340 BH, Neth.  
Recueil des Travaux Chimiques des Pays-Bas (1993), 112(12), 627-34  
CODEN: RTCPA3; ISSN: 0165-0513

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:270951

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

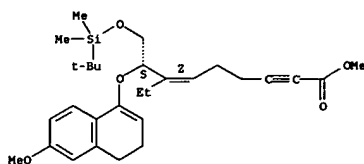
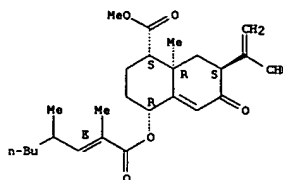
AB A total synthesis of the title compound I, a potential precursor of the progestagens desogestrel and 3-ketodesogestrel, is described. The backbone of the steroid was assembled by condensation of 1,2-dihydronaphthalene II with 6-nonen-2-ynoic acid III (TBDS = tert-butyldimethylsilyl) and subsequent Claisen rearrangement of the resulting enol ether to give disecosteroid IV. Heating of IV at 170° gave a 1:1 mixture of 9,11-secosteroids V and its 13a epimer. The 13a-epimer V was converted into 9,11-secogona-1,3,5(10)-triene-9,17-dione VI (X = Br), which was treated with triphenylphosphine under high pressure conditions (12 kbar, 55°) to give the corresponding phosphonium salt VII (X = P+Ph3 Br-) (VII). The intramolecular Wittig reaction of VII proceeded with epimerization at C-8 to give exclusively the 8a epimer of I, which underwent isomerization upon treatment with acid to the title compound I.

IT 154619-36-0P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (formation and Claisen rearrangement of)

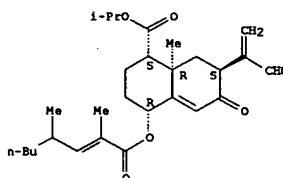
RN 154619-36-0 HCAPLUS

CN 6-Nonen-2-ynoic acid, 8-[[[(3,4-dihydro-6-methoxy-1-naphthalenyl)oxy]-9-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-ethyl-, methyl ester, (S-[2])-(9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, methyl ester, (1S,4R,7S,8aR)-(9CI) (CA INDEX NAME)Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.  
Currently available stereo shown.

RN 215866-74-3 HCAPLUS

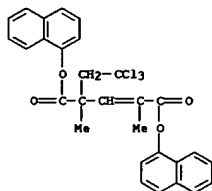
CN 1-Naphthalenecarboxylic acid, 4-[(2,4-dimethyl-1-oxo-2-octenyl)oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, 1-methylethyl ester, (1R,4S,7R,8aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.

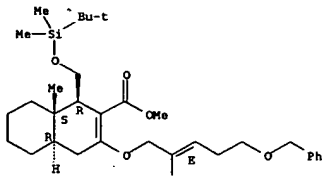
L8 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

10780391s2

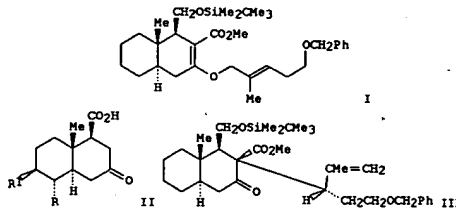
L8 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 21 Mar 1987  
 ACCESSION NUMBER: 1987:85169 HCAPLUS  
 DOCUMENT NUMBER: 106:85169  
 TITLE: Study on radical telomerization of esters of methacrylic acid by using bromotrichloromethane and characteristics of the resulting telomers. III. Aryl methacrylates  
 AUTHOR(S): Kimura, Takao; Nakanishi, Itaru; Hamashima, Motome  
 CORPORATE SOURCE: Fac. Eng., Utsunomiya Univ., Utsunomiya, 321, Japan  
 SOURCE: Polymer Journal (Tokyo, Japan) (1986), 18(10), 689-97  
 CODEN: POLJBB; ISSN: 0032-3896  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Radical telomerization of Ph (I), 1-naphthyl (II) and 2-naphthyl methacrylate (III) with BrCCl<sub>3</sub> as a telogen at 50, 70, and 90° gave similar product distributions and tacticity as those of Me methacrylate (IV), but without formation of lactones. The order of the apparent rate of telomerization was IV > I > II > III. The n[Monomer]:[BrCCl<sub>3</sub>] adducts, i.e., the n-mers (n = 1-3), were separated by silica gel column chromatog. The aryl methacrylate and IV telomers differed remarkably from each other in reactivity. The elimination reaction of the aromatic telomers with Et<sub>3</sub>N was labile and complicated in comparison with that of the IV telomers, and the dimers underwent main chain scission in addition to the normal elimination reaction. The catalytic lactonization of the aromatic dimers gave unsatd. compds. in preference to lactones, which were exclusively obtained in the pyrolysis of the IV dimers. Furthermore, the pyrolysis of the naphthyl methacrylate dimers resulted in the diastereoisomerization through depolymn.  
 IT 106749-91-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 106749-91-1 HCAPLUS  
 CN 2-Pentenedioic acid, 2,4-dimethyl-4-(2,2,2-trichloroethyl)-, di-1-naphthalenyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 15 Jun 1985  
 ACCESSION NUMBER: 1985:204128 HCAPLUS  
 DOCUMENT NUMBER: 102:204128  
 TITLE: Acyclic diastereoselection as a synthetic route to quassinoids: a Claisen rearrangement based strategy for bruceantin  
 AUTHOR(S): Ziegler, Frederick E.; Klein, Scott I.; Pati, Uttam K.; Wang, Tein Fu  
 CORPORATE SOURCE: Sterling Chem. Lab., Yale Univ., New Haven, CT, 06511, USA  
 SOURCE: Journal of the American Chemical Society (1985), 107(9), 2730-7  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 102:204128  
 GI



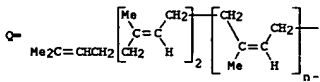
AB Claisen rearrangement of allyl vinyl ether I, prepared in many steps from the exocycliccarboxylic acid II (R = R<sub>1</sub> = H), gave the [(benzyloxy)ethyl]decalin derivative III having the correct stereo at C(8), C(9), and C(14) for quassinoids. Moreover, II (R = Me, R<sub>1</sub> = MeOCH<sub>2</sub>), a potential synthon for bruceantin, was also prepared  
 IT 95531-82-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and diastereoselective Claisen rearrangement of)  
 RN 95531-82-1 HCAPLUS  
 CN 2-Naphthalenecarboxylic acid, 1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1,4,4a,5,6,7,8,8a-octahydro-8a-methyl-3-[[[2-methyl-5-(phenylmethoxy)-2-pentenyl]oxy]-, methyl ester, [1R-[1a,3(E),4aB,8a]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

L8 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 23 Jun 1984  
 ACCESSION NUMBER: 1984:210218 HCAPLUS  
 DOCUMENT NUMBER: 100:210218  
 TITLE: Polyprenyl compounds  
 PATENT ASSIGNER(S): Kuraray Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.  
 CODEN: JKOJAF  
 Patent  
 DOCUMENT TYPE: Japanese  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

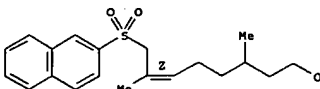
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58206554	A	19831201	JP 1982-90886	19820527
JP 03059058	B	19910909		

PRIORITY APPLN. INFO.: JP 1982-90886 19820527  
 GI



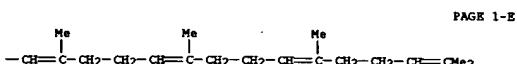
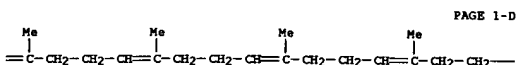
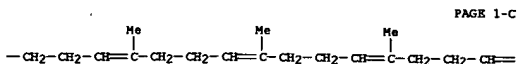
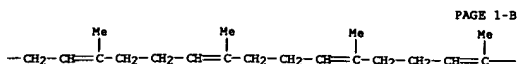
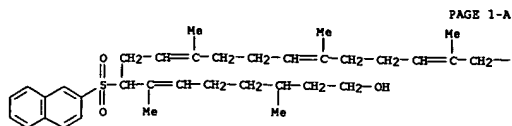
AB QCH<sub>2</sub>OMe:CHCH<sub>1</sub>CH<sub>2</sub>OMe:CHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OMeCH<sub>2</sub>CH<sub>2</sub>R [I, R = (protected) OH; R<sub>1</sub>, R<sub>2</sub> = H, 5(0)Me<sub>3</sub> where n = 0, 1, 2 and R<sub>3</sub> = alkyl, (halo) Ph, naphthyl, pyridyl, thiazolyl; n = 10-18] were prepared. Thus, QCH<sub>2</sub>OMe:CHCH<sub>2</sub>R<sub>4</sub> (II, R<sub>4</sub> = OH, n = 15), isolated from Pinus densiflora along with II (R<sub>4</sub> = CH<sub>3</sub>; n = 10-14, 16-18), was treated with HSP in DMF containing K<sub>2</sub>CO<sub>3</sub> to give II (R<sub>4</sub> = SPh, n = 15), whose oxidation gave II (R<sub>4</sub> = SO<sub>2</sub>Ph, n = 15), reaction of which (6.83 g) with 1.92 g BrCH<sub>2</sub>OMe:CHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OMeCH<sub>2</sub>CH<sub>2</sub>Q1 (Q1 = tetrahydropyran-2-yloxy) in THF containing (Me<sub>2</sub>N)3PO and BuLi at -10 to 0° for 1 h and then at 20° overnight gave 6.74 g I (R = tetrahydropyran-2-yloxy, R<sub>1</sub> = SO<sub>2</sub>Ph, R<sub>2</sub> = H, n = 15), deprotection of which in EtOH-HCl-H<sub>2</sub>O gave I (R = OH, R<sub>1</sub> = SO<sub>2</sub>Ph, R<sub>2</sub> = H, n = 15).  
 IT 90165-55-2  
 RL: RCT (Reactant); RACT (Reactant or reagent) (condensation of, with polyprenol derivs.)  
 RN 90165-55-2 HCAPLUS  
 CN 6-Octen-1-ol, 3,7-dimethyl-8-(2-naphthalenylsulfonyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

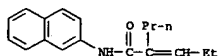


IT 90165-36-9P

L8 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 90165-36-9 HCAPLUS  
 CN 6,10,14,18,22,26,30,34,38,42,46,50,54,58,62,66,70,74,78-  
 Octacontanonadecan-1-ol, 3,7,11,15,19,23,27,31,35,39,43,47,51,55,59,63,67,  
 ,71,75,79-eicosamethyl-8-(2-naphthalenylsulfonyl)- (SCI) (CA INDEX NAME)



L8 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 α-Propyl-γ-methylbutyrolactone, b10 109°, hydrazide, m.  
 138°. α-Propyl-β-γ-pentenic chloride, b10  
 66-7°; anilide, m. 72°; β-naphthylamide, m.  
 117°. Ethyl α-brom-α-propyl-n-valerate, b8  
 99-100°, may be prepared by action of Br on the chloride of  
 dipropylacetic acid. By treating this ester with diethylaniline, one  
 obtains an unsaturated ester, b8 76-77°, which on saponification  
 gives α-propyl-β-ethylacrylic acid (stable) m. 36°.  
 There is a little of the unstable form produced at the same time. Ethyl  
 ester (of stable form), b10 83°. Acid chloride, b9 74°.  
 Anilide, m. 68°. β-Naphthylamide, m. 89°. The  
 unstable form may be transformed into stable form by conversion into the  
 acid chloride by PCl3 and subsequent treatment with pyridine.  
 IT 861069-80-9, α-Pentenamide, N-2-naphthyl-α-propyl-  
 (two)  
 RN 861069-80-9 HCAPLUS  
 CN α-Pentenamide, N-2-naphthyl-α-propyl- (ICI) (CA INDEX NAME)



L8 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ED Entered STN: 16 Dec 2001  
 ACCESSION NUMBER: 1908:3432 HCAPLUS  
 DOCUMENT NUMBER: 2:3432  
 ORIGINAL REFERENCE NO.: 2:801F-1,802a-e  
 TITLE:--  
 Stereoisomerism in the Group of the Unsaturated  
 α,β-Acyclic Acids  
 Blaise, E.; Bagard, P.  
 SOURCE: Ann. chim. phys. [8] (1908), 11(III)  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 GI For diagram(s), see printed CA Issue.

AB The action of heat on tertiary α-hydroxyacids gives a small quantity  
 of the ketones, but principally the unsaturated add. The ketone  
 diminishes, while the unsaturated acid increases in quantity with rising  
 molecular weight. In some cases lactides are formed. Whenever  
 stereoisomeric forms of the unsaturated acid are possible, it is the  
 unstable isomer which is produced. With rise in molecular weight the  
 unstable isomers show greater stability toward influences which tend to  
 bring about their isomerization into the stable form.  
 α-Hydroxy-α-methylpropionic acid gives about 30% of its lactide  
 Me2C - CO - O, 13% methylacrylic add and 48% acetone.  
 α-Hydroxy-α-methylbutyric acid gives about 10%  
 methylacetylketone, 17% angelic acid, 18% tiglic and 25% of the lactide, m.  
 29°. Anilide of angelic acid, by action of EtMgBr on aniline and  
 ethyl angelate, crystallized from benzene, m. 126°.  
 β-naphthylamide, Me.CH: CMeCONHC10H7, by a method similar to that for  
 the anilide, m. 135°. Anilide of tiglic acid, from aniline and  
 tiglyl, chloride, m. 77°, β-naphthylamide, m. 96°.  
 α-Hydroxyethylbutyric acid on being heated gives a little  
 diethylketone, whose semicarbazone m. 139° and α-ethyl-β-  
 methylacrylic acid, MeCH: CMeCO2H, b. 107-8°, m. -35°  
 different from the stable isomer described by Fittig (Ann., 268, 22). No  
 lactide was formed from the α-hydroxyethylbutyric acid. From  
 α-ethyl-β-methylacrylic acid (labile) were prepared copper,  
 zinc, and cadmium salts; ethyl ester, b0 52°; anilide, m.  
 97°; β-naphthylamide, m. 127°; and a dibromide, m.  
 109°. α-Ethyl-β-methylacrylic acid (stable) (Frankland  
 and Duppa, Ann., 136, 2, and Fittig, Ann., 268, 22) by dehydration by P2O5  
 and saponification of the ethyl α-ethyl-β-hydroxybutyrate  
 obtained by action of Zn and acetaldehyde on ethyl α-bromobutyrate,  
 m. 45°, b13 109°. From this acid were obtained the acid  
 chloride, b13 54°; anilide, m. 95°; β-naphthylamide, m.  
 96°; and the copper and zinc salts. The labile form of the acid  
 can be changed into the stable form by the action of halogen acids, as  
 HBr, or by forming the acid chloride by means of PCl3 and treatment of  
 this with pyridine. From the products of distillation of  
 α-propyl-α-oxy-n-valeric acid were obtained 2% dipropylketone,  
 giving semicarbazone m. 133°, 58% α-propyl-β-  
 ethylacrylic add (unstable), 5% α-propyl-β-γ-pentenic  
 acid, 5% α-propyl-γ-methylbutyrolactone, giving a hydrazone.  
 From α-propyl-β-ethylacrylic add (unstable) the calcium salt;  
 ethyl ester, b10 77-8°; anilide m. 40-1°; and  
 β-naphthylamide m. 104°, were prepared. Dehydration by means  
 of P2O5, of either ethyl α-hydroxy-α-propyl-n-valerate or  
 ethyl β-hydroxy-α-propyl-n-valerate, b8 105°, gave  
 α-propyl-β-γ-pentenic acid, b10 120-1°.

10780391s2

=> log y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
108.00	466.00
SINCE FILE	TOTAL
ENTRY	SESSION
-15.60	-17.16

STN INTERNATIONAL LOGOFF AT 11:19:14 ON 05 JAN 2007

10780391s1

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANAG1626

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'REGISTRY' AT 09:39:17 ON 05 JAN 2007  
FILE 'REGISTRY' ENTERED AT 09:39:17 ON 05 JAN 2007  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	346.00	346.21

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	346.00	346.21

FILE 'REGISTRY' ENTERED AT 09:39:31 ON 05 JAN 2007  
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STRUCTURE FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1  
DICTIONARY FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

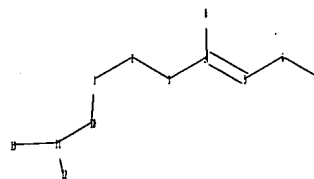
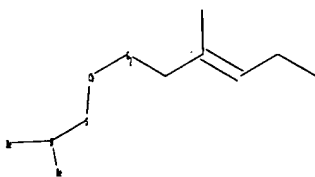
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10780391ss1.str

10780391s1



chain nodes :

1 2 3 4 5 6 7 8 10 11 12 13

chain bonds :

1-2 1-10 2-3 3-4 4-5 4-8 5-6 6-7 10-11 11-12 11-13

exact/norm bonds :

1-2 2-3 10-11

exact bonds :

1-10 3-4 4-5 4-8 5-6 6-7 11-12 11-13

G1:O,S

G2:O,S,N

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS

Generic attributes :

1:

Saturation : Unsaturated

Type of Ring System : Polycyclic

Element Count :

Node 1: Limited

C,C10

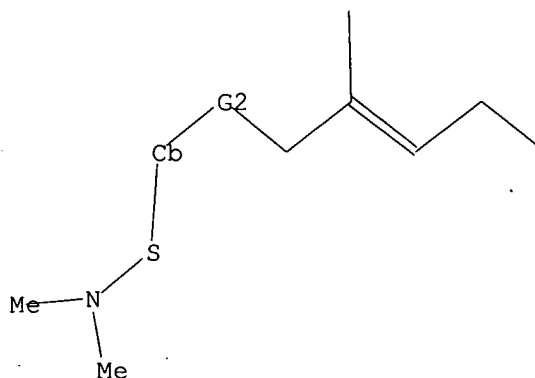
10780391s1

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



G1 O,S

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 09:40:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 26 TO ITERATE

100.0% PROCESSED 26 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 215 TO 825

PROJECTED ANSWERS: 1 TO 80

L8 1 SEA SSS SAM L7

=> s 17 full

FULL SEARCH INITIATED 09:40:09 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 458 TO ITERATE

100.0% PROCESSED 458 ITERATIONS

11 ANSWERS

SEARCH TIME: 00.00.01

L9 11 SEA SSS FUL L7

=> fil hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

518.31

FILE 'HCAPLUS' ENTERED AT 09:40:15 ON 05 JAN 2007

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FILE COVERS 1907 - 5 Jan 2007 VOL 146 ISS 3  
FILE LAST UPDATED: 4 Jan 2007 (20070104/ED)

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=> s 19

L10 2 L9

=> d ed ibib abs hitstr 1-2



10780391s1

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 05 Oct 2004

ACCESSION NUMBER: 2004:807711 HCAPLUS

DOCUMENT NUMBER: 142:6669

TITLE: Synthesis and Activity of Fluorescent Isoprenoid Pyrophosphate Analogs  
 AUTHOR(S): Kim, Heekyoung; Kleckley, Troy S.; Wiener, Andrew J.; Holstein, Sarah A.; Hohl, Raymond J.; Wiener, David F.

CORPORATE SOURCE: Departments of Chemistry Pharmacology and Internal Medicine, University of Iowa, Iowa City, IA, 52242-1294, USA  
 SOURCE: Journal of Organic Chemistry (2004), 69(24), 8186-8193

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:6669

AB New fluorescent analogs of farnesol and geranylgeraniol were prepared and then converted to the corresponding pyrophosphates. These analogs incorporate anthranilate or dansyl-like groups anchored to the terpenoid skeleton through amine bonds that would be expected to be relatively stable to metabolism. After addition of the alcs. or the pyrophosphates

to the culture medium, their fluorescence is readily observed inside a human-derived leukemia cell line. Enzyme assays have revealed that the farnesyl pyrophosphate analog is an inhibitor of Ffase, while the corresponding alc. is not. These results, together with Western blot analyses of cell lysates, indicate that the farnesyl pyrophosphate analog penetrates the cells as an intact pyrophosphate and that it does so at a biol. relevant concentration.

IT 491861-22-4P  
 RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

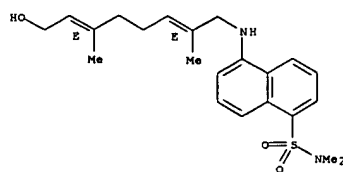
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)

RN 491861-22-4 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

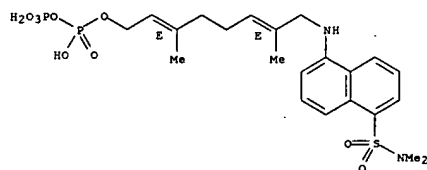


IT 798573-69-0P  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)

RN 798573-69-0 HCAPLUS

CN Diphosphoric acid, mono-[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester, triammonium salt (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● 3 NH3

IT 798573-65-6P 798573-66-7P 798573-68-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

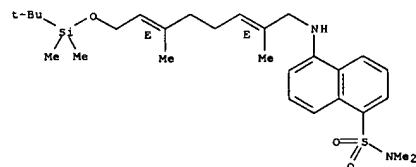
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)

RN 798573-65-6 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-[[[1,1-dimethylethyl]dimethylsilyloxy]-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

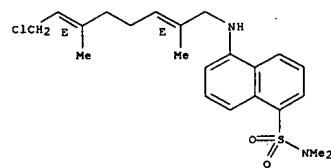
Double bond geometry as shown.



RN 798573-66-7 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-chloro-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 798573-68-9 HCAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, (2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl (diphosphate) (3:1) (9CI) (CA INDEX NAME)

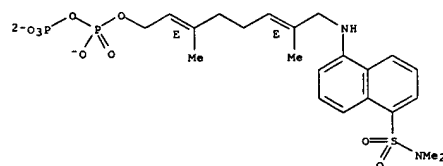
CM 1

CRN 798573-67-8

CMF C22 H29 N2 O9 P2 S

Double bond geometry as shown.

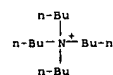
L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 10549-76-5

CMF C16 H36 N



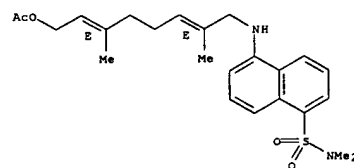
IT 798573-64-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)

RN 798573-64-5 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-(acetyloxy)-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 31 Jan 2003

ACCESSION NUMBER: 2003:77548 HCAPLUS

138:142470

DOCUMENT NUMBER: Isoprenoid analog compounds and methods of making and

TITLE: use thereof

INVENTOR(S): Wiemer, David; Hohl, Raymond J.

PATENT ASSIGNEE(S): University of Iowa Research Foundation, USA

SOURCE: U.S. Pat. Appl. Publ., 18 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003022869	A1	20030130	US 2002-116737	20020403
US 6727234	B2	20040427		
US 2004167102	A1	20040826	US 2004-780391	20040217
PRIORITY APPLN. INFO.:			US 2001-281170P	P 20010403
			US 2002-116737	A3 20020403

OTHER SOURCE(S): MARPAT 138:142470

AB The invention provides isoprenoid compds. and their pharmaceutically acceptable salts useful, for example, for blocking prenylation

transferase enzymes, for probing or diagnosing protein prenylation processes, and for treating cancer in a mammal. A method of accessing the metabolic status of an enzyme comprises (a) contacting the enzyme with an effective

amount of a mixture of a farnesol analog compound and a geraniol or geranylgeraniol analog compound, and (b) measuring the relative ratio of farnesylation to geranylgeranylation of the farnesol and the geraniol or geranylgeraniol analog compds. accomplished by the enzyme. The invention also provides pharmaceutical compns., and processes for preparing isoprenoid compds.

and

their intermediates.

IT 491861-20-2P

RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation);

THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(isoprenoid analog compds. for diagnosis and treatment of cancer)

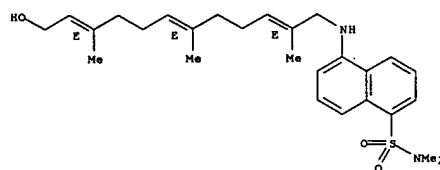
RN 491861-20-2 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E,10E)-12-hydroxy-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



IT 491861-19-9P 491861-21-3P 491861-22-4P

491861-23-5P

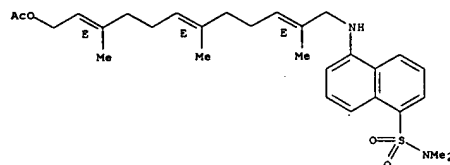
RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(isoprenoid analog compds. for diagnosis and treatment of cancer)

RN 491861-19-9 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E,10E)-12-(acetyloxy)-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

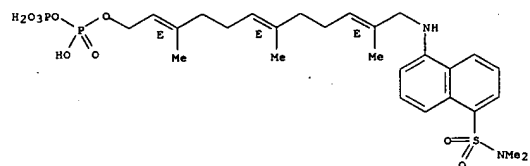


RN 491861-21-3 HCAPLUS

CN Diphosphoric acid, mono[[[(2E,6E,10E)-12-[[5-[[[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7,11-trimethyl-2,6,10-dodecatrienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

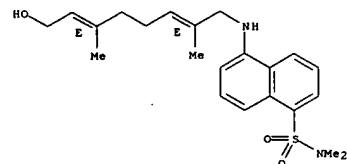
L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 491861-22-4 HCAPLUS

CN 1-Naphthalenesulfonamide, 5-[[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

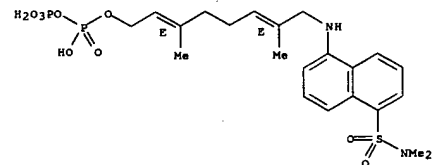
Double bond geometry as shown.



RN 491861-23-5 HCAPLUS

CN Diphosphoric acid, mono[[[(2E,6E)-8-[[5-[[[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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=> log y

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

13.14

531.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

ENTRY

TOTAL

SESSION

CA SUBSCRIBER PRICE

-1.56

-1.56

STN INTERNATIONAL LOGOFF AT 09:40:46 ON 05 JAN 2007